



# EMERGING SCIENCE FOR ENVIRONMENTAL HEALTH DECISIONS

## AGENDA

### Applying 21st Century Toxicology to Green Chemical and Material Design

SEPTEMBER 20-21, 2011 ■ TUESDAY 8:30-5:00, WEDNESDAY 8:30-NOON\*  
HOUSE OF SWEDEN EVENT CENTER, 2900 K STREET NW, WASHINGTON, DC

**MORE THAN 83,000 CHEMICALS** are available for use in the U.S. today, many of which pose serious hazards to the environment and human health. The rising concern about toxic properties of chemicals has given rise to the field of “green chemistry”—the science-based design of chemicals, chemical processes, and products that minimize the use and generation of hazardous substances. Green chemistry, based upon 12 fundamental principles<sup>1</sup>, takes a life-cycle approach where each chemical is evaluated from its “birth (i.e., development and production) through its ultimate disposal after use. Thinking up front about what substances are used to make chemicals, how a chemical may be transformed in biological and environmental

systems, and how and where a chemical is transported in those systems may help shift society’s paradigm from one of hazard or risk response to a paradigm of hazard and risk prevention.

**NEW TOXICOLOGICAL TESTING METHODS** and tools are emerging that hold real potential to facilitate rapid screening of large numbers of chemicals for their inherent biological and environmental characteristics. Use of such methods and tools to inform chemical design and synthesis is one exciting area of potential application. However, a true understanding and evaluation of biological responses and toxicology has yet to be well-incorporated into the chemical design process.

**THIS WORKSHOP WILL BRING CHEMISTS, TOXICOLOGISTS, INDUSTRY** sustainability and executive officers, and other scientists and stakeholders together to define common goals, identify knowledge gaps, and promote applied research aimed at expediting and targeting the application of this “new toxicology” to the emerging field of green chemistry with its life cycle approach. The workshop will begin with an overview of green chemistry and stakeholder perspectives on current efforts and needs for accelerating green-chemical design. Presentations and discussions will also explore different rapid assessment approaches in toxicology, including high-throughput biochemical screening, in vitro cellular approaches, and rapid assessments using aquatic organisms. Such questions as “how can early consideration of toxicological factors assist with chemical design?” and

*(continued)*

<sup>1</sup> “The 12 Principles of Green Chemistry” United States Environmental Protection Agency. <http://www.epa.gov/gcc/pubs/principles.html>. Retrieved 2 June 2011

The origin of this workshop topic was the Toxics and Risk Subcommittee (T&R) of the National Science and Technology Council’s Committee on Environment, Natural Resources, and Sustainability. T&R is comprised of senior representatives from 16 federal agencies and seeks to coordinate federal science and technology efforts related to the identification, prevention, and mitigation of problems arising from human and non-human exposure of to potentially toxic materials. One focus is on how advances in molecular and computational methods in toxicology (e.g., high-throughput screening) can facilitate green chemical design.

Through the NIEHS role as T&R co-chair and sponsor of the NAS standing committee, the topic was advanced and found to be of mutual interest to the NAS and the Emerging Science Committee.

\* On Wednesday, September 21, the committee and liaisons will meet until 3:00pm.

“what toxicology factors are important?” will be discussed. Presenters will highlight design and production considerations in new materials and chemicals like nanomaterials, pesticides, and oil dispersants to demonstrate how advancing toxicological testing approaches might be incorporated into the emerging field of green chemistry. Particular attention will be given to the

relative advantages and limitations of the emerging rapid assessment approaches and how the data can be used to inform green chemistry decisions. This important and timely synthesis will allow the exchange of knowledge and experiences to identify a path forward for establishing the next generation of safer chemicals to better protect human health and the environment.

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## TUESDAY, SEPTEMBER 20, 2011 (8:30AM–5PM)

- 8:30 Opening Remarks—Linda Birnbaum, *National Institute of Environmental Health Sciences*
- 8:35 Workshop Objectives—Richard Denison<sup>†</sup>, *Environmental Defense Fund*

### SESSION 1 VISION AND PERSPECTIVES

Session 1 will include a short primer on the principles of green chemistry and a vision for how emerging toxicological testing tools can be integrated into green chemical and product design. This session will also layout industry perspectives and vision about toxicology for use in a life-cycle approach to green chemical design.

Session Chair: Richard Denison<sup>†</sup>, *Environmental Defense Fund*

- 8:45 Vision for a Green Chemical Future—Paul Anastas, *U.S. Environmental Protection Agency (EPA)*
- 9:15 Incorporating Green Chemistry Concepts into New Product R&D—Mark Thompson, *DuPont*
- 9:45 Manufacturing Green Products—Helen Holder, *Hewlett-Packard*
- 10:15 Break

### SESSION 2 RAPID HAZARD ASSESSMENT TESTING APPROACHES

Session 2 will outline rapid toxicity testing approaches and chemical structural analyses that may be useful in green chemical design. Concrete examples of how rapid approaches are being used or integrated will be highlighted.

Session Chair: Ivan Rusyn<sup>†</sup>, *University of North Carolina (UNC), Chapel Hill*

- 10:25 Application of Rapid In Vivo Approaches to Green Chemistry—Robert Tanguay, *Oregon State University*

- 10:55 Application of Rapid In Vitro ToxCast Assays to Green Chemical Design—David Dix, *EPA*

- 11:25 The Role of Holistic Assay Platforms and Computational Methods to Prioritize Pharmaceutical Candidates—Russell Naven, *Pfizer*

- 12:00 Lunch on your own

- 1:15 Development of Molecular Design Guidelines for Reduced Toxicity—Adelina Voutchkova, *Yale University*

- 1:45 Cheminformatics and High-throughput Screening to Improve Toxicity Prediction—Alex Tropsha, *UNC, Chapel Hill*

- 2:15 Level of Confidence for Current and Future Uses of Rapid Toxicity Testing Approaches—Edward Carney, *The Dow Chemical Company*

- 2:45 Break

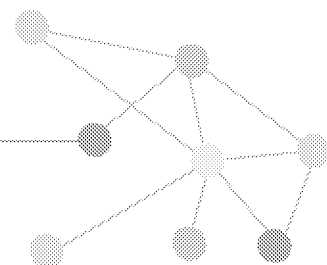
- 3:00– Session 2 Panel Discussion

- 5:00
- Testing Considerations in the Development of Green Nanomaterials
  - Broad Discussion of Testing Approaches for Green Chemicals and Materials

Moderator: William Farland<sup>†</sup>, *Colorado State University*

Panelists: Richard Denison<sup>†</sup>, *Environmental Defense Fund*; Jim Hutchinson, *University of Oregon*; Mark Thompson, *DuPont*; Harold (Hal) Zenick, *EPA*; Session 2 Speakers

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## WEDNESDAY, SEPTEMBER 21 (8:30AM-NOON)

8:30 Welcome to Day 2—Lauren Zeise<sup>†</sup>, *California Environmental Protection Agency (CalEPA)*

### SESSION 3 PRACTICAL APPROACHES, BALANCING CONSIDERATIONS, AND NEXT STEPS

Session 3 will focus on U.S. and international thinking and frameworks to integrate rapid testing into the chemical design process. This session will also focus on the broader considerations and how to balance chemists' understanding, toxicologists' perspectives, and industry needs.

Session Chair: Lauren Zeise<sup>†</sup>, *CalEPA*

8:35 Defining Safer Chemicals: Implications of New Test Methods for Current Frameworks—Cal Baier-Anderson, *EPA*

<sup>†</sup> indicates a member of the Standing Committee on Use of Emerging Science for Environmental Health Decisions.

Please note that this meeting will be webcast and recorded. Please visit our website for webcast details.

9:05 The Use of New Toxicological Tools within a Chemical Risk Assessment Framework: A European Perspective—Sharon Munn, *Institute for Health and Consumer Protection, Italy*

9:35 Bridging Considerations—Tom Osimitz, *Science Strategies*

10:05 Break

10:15– Panel Discussion

11:45 Panelists: Kathryn Guyton, *EPA*; Helen Holder, *Hewlett-Packard*; Mark Johnson, *U.S. Army Public Health Command*; Jennifer Sass, *Natural Resources Defense Council*; Thaddeus Schug, *NIEHS*; Session 3 Speakers

11:45 Workshop Summary—William Farland<sup>†</sup>, *Colorado State University*

12:00 Workshop Adjourns (post-workshop Committee and Liaison meetings until 3:00 pm)

### SAVE THESE DATES—

■ Dec. 8–9, 2011 *Emerging Technologies for Measuring Individual Exposomes*

■ Apr. 18–19, 2012 *Individual Variability*

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<http://dels.nas.edu/envirohealth>

Emerging Science workshops are free and open to the public.

### About the Committee

At the request of the National Institute of Environmental Health Sciences (NIEHS), the National Research Council formed the Standing Committee on Use of Emerging Science for Environmental Health Decisions to facilitate communication among government, industry, environmental groups, and the academic community about scientific advances that may be used in the identification, quantification, and control of environmental impacts on human health.

